Eclipsed Acetaldehyde as a Precursor for Producing Vinyl Alcohol

By: Osman, OI (Osman, Osman I.); Alyoubi, AO (Alyoubi, Abdulrahman O.); Elroby, SAK (Elroby, Shabaan A. K.); Hilal, RH (Hilal, Rifaat H.); Aziz, SG (Aziz, Saadullah G.)

View ResearcherID and ORCID

INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES
Volume: 13 Issue: 11 Pages: 15360-15372
DOI: 10.3390/ioms131115360
Published: NOV 2012
View Journal Impact

Abstract
The MP2 and DFT/B3LYP methods at 6-311++ G(d,p) and aug-cc-pdz basis sets have been used to probe the origin of relative stability preference for eclipsed acetaldehyde over its bisected counterpart. A relative energy stability range of 1.02 to 1.20 kcal/mol, in favor of the eclipsed conformer, was found and discussed. An NBO study at these chemistry levels complemented these findings and assigned the eclipsed acetaldehyde preference mainly to the vicinal antiperiplanar hyperconjugative interactions. The tautomeric interconversion between the more stable eclipsed acetaldehyde and vinyl alcohol has been achieved through a four-membered ring transition state (TS). The obtained barrier heights and relative stabilities of eclipsed acetaldehyde and the two conformers of vinyl alcohol at these model chemistries have been estimated and discussed.

Keywords
Author Keywords: acetaldehyde; eclipsed; bisected; vinyl alcohol; tautomerization; hyperconjugation; MP2; B3LYP; NBO
KeyWords Plus: HYDROXYETHYLIDENE CH3-C-OH; MICROWAVE-SPECTRUM; DIPOLE-MOMENT; ACETONE

Author Information
Reprint Address: Osman, OI (reprint author)

Organization-Enhanced Name(s)
King Abdulaziz University

Addresses:
Organization-Enhanced Name(s)
King Abdulaziz University

E-mail Addresses: oabdElkarim@kau.edu.sa; aalyoubi@kau.edu.sa; skamel@kau.edu.sa; rhilal@kau.edu.sa; saaziz@kau.edu.sa

Funding

<table>
<thead>
<tr>
<th>Funding Agency</th>
<th>Grant Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>King Abdulaziz University, Jeddah</td>
<td>D7-130/1432</td>
</tr>
<tr>
<td>DSR</td>
<td></td>
</tr>
</tbody>
</table>

Citation Network
2 Times Cited
28 Cited References
View Related Records
Create Citation Alert
(data from Web of Science Core Collection)

All Times Cited Counts
2 in All Databases
2 in Web of Science Core Collection
0 in BIOSIS Citation Index
0 in Chinese Science Citation Database
0 in Data Citation Index
0 in Russian Science Citation Index
0 in SciELO Citation Index

Usage Count
Last 180 Days: 0
Since 2013: 21
Learn more

Most Recent Citation
Hussein, M. A. Photoactivity, Optical Behavior and DFT Studies of 2,5-Bis[4-chloro-acetyl](thiophen-2-ylmethylene)cyclopentanone BCTCP in Different Solvents. JOURNAL OF FLUORESCENCE, MAY 2017.
View All

This record is from:
Web of Science Core Collection
- Science Citation Index Expanded

Suggest a correction
If you would like to improve the quality of the data in this record, please suggest a correction.